

=> d his

(FILE 'HOME' ENTERED AT 10:35:52 ON 29 NOV 2006)

FILE 'CA' ENTERED AT 10:36:01 ON 29 NOV 2006

L1 1998 S (PH OR ACID? OR BASE OR DEPROTONA?) (3A) (DEPEND? OR VARIAB? OR
VARY? OR INSTABIL? OR SENSITIV?) (8A) FLUORESC?
L2 23 S L1 AND (LABIL? (2A) (HYDROGEN OR H OR PROTON) OR METHYLAT? OR
ETHYLAT? OR ALKYLA?)

=> d bib,ab 12 1-23

L2 ANSWER 8 OF 23 CA COPYRIGHT 2006 ACS on STN
AN 129:181947 CA
TI UV/Vis and fluorescence study on anthralin and its **alkylated** derivatives
AU Sellmer, Andreas; Terpetschnig, Ewald; Wiegrebe, Wolfgang; Wolfbeis,
Otto S.
CS Dep. Pharm. Chem. I, Univ. Regensburg, Regensburg, D-93040, Germany
SO Journal of Photochemistry and Photobiology, A: Chemistry (1998), 116(1),
39-45
AB Anthralin and some of its C-10 or O-**alkylated** derivs. were investigated
by UV/VIS- and fluorescence spectroscopy in different solvents and
buffer systems, resp. The effects of substituents on the formation of
anthralin anion as well as the constitution of the resulting anions
confirm that C-H acidity at position 10 is necessary for the formation
of a fully arom. anionic form. It is concluded that the resulting anion
is the pharmacol. active species of the antipsoriatic anthralin.
Tautomerism of the neutral mol. is not observable.

L2 ANSWER 14 OF 23 CA COPYRIGHT 2006 ACS on STN
AN 118:191020 CA
TI Fluorescent species of 7-azaindole and 7-azatryptophan in water
AU Chen, Y.; Rich, R. L.; Gai, F.; Petrich, J. W.
CS Dep. Chem., Iowa State Univ., Ames, IA, 50011, USA
SO Journal of Physical Chemistry (1993), 97(9), 1770-80
AB A study of the fluorescence lifetimes and quantum yields of 7-azaindole
and its **methylated** derivs. N1-methyl-7-azaindole (1M7AI) and 7-methyl-
7H-pyrrolo[2,3-b]pyridine (7M7AI) in water is performed in order to
explain the observation that the fluorescence spectrum of 7-azaindole
apparently consists of one band (λ_{max} = 386 nm) whereas in alcs. the
spectrum is bimodal (e.g., for methanol, λ_{max} = 374, 505 nm). Careful
measurements of the fluorescence decay as a function of emission
wavelength indicate a small amplitude of an ≈ 70 -ps decaying component at
the bluer wavelengths and a rising component of the same duration at the
redder wavelengths. The small amplitude component, which comprises no
more than 20% of the fluorescence decay, is attributed to excited-state
tautomerization that is mediated by the solvent. Particular attention
is paid to the **pH dependence** of the **fluorescence** lifetimes and yields.
Upon tautomerization, the basic 1-nitrogen (N1) of 7-azaindole is
rapidly protonated giving rise to a species whose emission max. is at \approx
440 nm. The fluorescence emission max. and lifetime of 7-azaindole is
dominated by the 80% of the solute mols. that are blocked by unfavorable
solvation from executing excited-state tautomerization. It is proposed
that ≈ 10 ns is required for the surrounding water mols. to
attain a configuration about 7-azaindole that is propitious for

tautomerization.

=> log y

STN INTERNATIONAL LOGOFF AT 10:46:24 ON 29 NOV 2006

=> d his

(FILE 'HOME' ENTERED AT 08:37:41 ON 29 NOV 2006)

FILE 'REGISTRY' ENTERED AT 08:37:51 ON 29 NOV 2006

L1 STRUCTURE UPLOADED

L2 50 S L1

L3 1656 S L1 FULL

FILE 'CA' ENTERED AT 08:39:29 ON 29 NOV 2006

L4 741 S L3

L5 23 S L4 AND FLUORESC?

L6 7 S L5 AND PY<2000

L7 25 S L4 AND PROTON?

L8 22 S L7 AND PY<2000

L9 29 S L6,L8

=> d 19 bib,ab,kwic 1-29

L9 ANSWER 8 OF 29 CA COPYRIGHT 2006 ACS on STN

AN 112:235234 CA

TI Chemistry of benzotriazoles. Benzotriazol-1-ylmethyammonium salts synthesis and reactivity

AU Katritzky, Alan R.; Hughes, Craig V.; Rachwal, Stanislaw

CS Dep. Chem., Univ. Florida, Gainesville, FL, 32611, USA

SO Journal of Heterocyclic Chemistry (1989), 26(6), 1579-88

AB Benzotriazol-1-ylmethyammonium salts on treatment with alkylating agents afford benzotriazol-1-ylmethyammonium salts e.g., I (R = Me, Et), also available from reactions of chloromethylbenzotriazole with tertiary amines. In deuterated solvents under basic conditions the methylene protons of these salts exchange with deuterium. At elevated temps., an alkyl group substituent migrated from the ammonium center to the benzotriazolyl N-3. Reaction of the salts with Grignard reagents afforded various products arising from substitution of the ammonium moiety and/or from attack on the benzotriazolyl N-3 or on the benzenoid ring.

IT 13351-73-0P 16584-05-7P 69218-29-7P 127236-93-5P

L9 ANSWER 10 OF 29 CA COPYRIGHT 2006 ACS on STN

AN 111:133584 CA <<LOGINID::20061129>>

TI Tautomerism and aromaticity in 1,2,3-triazoles: the case of benzotriazole

AU Tomas, Francisco; Abboud, Jose Luis M.; Laynez, Jose; Notario, Rafael; Santos, Lucia; Nilsson, Sven Ove; Catalan, Javier; Claramunt, Rosa Maria; Elguero, Jose

CS Fac. Cienc., Univ. Valencia, Valencia, Spain

SO Journal of the American Chemical Society (1989), 111(19), 7348-53

AB This paper provides an explanation for the extraordinary difference in stability between 1,2,3-triazole and benzotriazole tautomers. In the gas phase, the 2H tautomer of 1,2,3-triazole represents more than 99.9% of the equil. mixt.; in benzotriazole the reverse is true (more than

99.99% of 1H tautomer at equil.). To understand the origin of this different behavior, an ab initio study at the 6-31G level was carried out on both tautomers of benzotriazole, on benzotriazolate anion, and on both tautomers of benzotriazolium cation (the 1,2- and the 1,3-H,H⁺ ions). Theor. results (the proton affinity of 1H-benzotriazole is 10.2 kcal mol⁻¹ larger than that of 2H-benzotriazole) were checked against ICR measurements with excellent agreement (1-methylbenzotriazole is 10.4 kcal mol⁻¹ more basic than 2-methylbenzotriazole). Thermodyn. measurements (enthalpies of soln., vaporization, sublimation, and solvation) in three solvents (water, methanol, and DMSO) confirm the predominance of the 1H tautomer in soln. Taking into account lone pair/lone pair repulsions and aromaticity, it is possible to explain the different behavior of 1,2,3-triazole and benzotriazole in the case of neutral mols. and their similarity in the case of protonated species.

IT 13351-73-0, 1-Methylbenzotriazole

L9 ANSWER 15 OF 29 CA COPYRIGHT 2006 ACS on STN

AN 95:50166 CA

TI Kinetics and mechanism of acid and base hydrolysis of cis-chloro (benzotriazole)bis(ethylenediamine)cobalt(III) and cis-chloro(N-methylbenzotriazole)bis(ethylenediamine)cobalt(III) cations

AU Rao, B. Seshagiri; Nanda, Rabindranath; Tripathy, Kumuda Kanta

CS Dep. Chem., Ravenshaw Coll., Cuttack, 753003, India

SO Transition Metal Chemistry (Dordrecht, Netherlands) (1981), 6(2), 97-100

AB The kinetics of acid hydrolysis of Cis-[CoCl(btzH)(en)₂]²⁺ and cis-[CoCl(btzMe)(en)₂]²⁺ complexes (where btzH = benzotriazole, btzMe = N-methylbenzotriazole and en = ethylenediamine) was studied in HClO₄ at ionic strength I = 0.25 mol dm⁻³ at 30-40°. In the 1.0 X 10⁻¹-1.0 X 10⁻³ mol dm⁻³ acid strength range, the rate of aquation of the [CoCl(btzH)(en)₂]²⁺ cation follows the relationship: -dln[complex]/dt = k₁ + k₂KNH [H⁺]⁻¹, where k and k₂ are aquation rate consts. of the acid independent and acid-dependent steps, resp., and KNH is the acid dissocn. const. of the coordinated benzotriazole. cis-[CoCl(btzMe)-(en)₂]²⁺ undergoes acid-independent hydrolysis presumably due to the absence of a labile N-H proton. The base hydrolysis could be followed for the cis-[CoCl(btzMe)(en)₂]²⁺ complex only by measuring hydrolysis rates at 0°.

IT 77968-02-6 (hydrolysis of, kinetics and mechanism of acid and base)

=> log y

STN INTERNATIONAL LOGOFF AT 08:45:09 ON 29 NOV 2006

=> d his

(FILE 'HOME' ENTERED AT 15:33:11 ON 28 NOV 2006)

FILE 'REGISTRY' ENTERED AT 15:33:21 ON 28 NOV 2006

L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED

L3 1 S L1-2

L4 17 S L1-2 FULL

FILE 'CA' ENTERED AT 15:36:10 ON 28 NOV 2006

L5 10 S L4

=> d 15 bib,ab,it 1-10

L5 ANSWER 1 OF 10 CA COPYRIGHT 2006 ACS on STN
AN 133:150218 CA
TI Fluorescent indicators for nitric oxide
AU Kojima, Hirotatsu; Nagano, Tetsuo
CS Graduate School of Pharmaceutical Sciences, The University of Tokyo,
Tokyo, 113-0033, Japan
SO Advanced Materials (Weinheim, Germany) (2000), 12(10), 763-765
AB Thus the authors have developed novel diamine fluorescent indicators
that enable real-time visualization of the prodn. and diffusion of NO in
living cells.
IT 287485-98-7

L5 ANSWER 3 OF 10 CA COPYRIGHT 2006 ACS on STN
AN 128:151321 CA
TI Development of a fluorescent indicator for the bioimaging of nitric
oxide
AU Kojima, Hirotatsu; Sakurai, Kuniko; Kikuchi, Kazuya; Kawahara,
Shigenori; Kirino, Yutaka; Nagoshi, Hiroshi; Hirata, Yasunobu; Akaike,
Takaaki; Maeda, Hiroshi; Nagano, Tetsuo
CS Graduate School of Pharmaceutical Sciences, University of Tokyo, Tokyo,
113, Japan
SO Biological & Pharmaceutical Bulletin (1997), 20(12), 1229-1232
AB Nitric oxide (NO) has been reported to play various roles as a signal
transmitter. However, detailed functions of NO have yet to be
clarified. A fluorescent indicator for NO imaging in living cells was
developed. The N-nitrosation of newly designed and synthesized 4-((3-
amino-2-naphthyl)aminomethyl)benzoic acid (DAN-1) by NO yielded the
highly fluorescent triazole-form. The membrane permeable ester deriv.
of DAN-1 (DAN-1 EE) was applied to the imaging of NO produced in
activated rat aortic smooth muscle cells. After DAN-1 EE has been
loaded into cells, the ester bond is hydrolyzed by intracellular
esterase, yielding original DAN-1 with less permeability. The
fluorescence intensity of the cells loaded with DAN-1 EE increased
according to NO prodn. The imaging method with fluorescent indicators
will be significant for the functional clarification of NO in vivo.
IT 202582-08-9P development of a fluorescent indicator for bioimaging of
nitric oxide)
(see also same journal 1998, 21, 1247) QP501, B566

L5 ANSWER 10 OF 10 CA COPYRIGHT 2006 ACS on STN
AN 29:28304 CA
OREF 29:3674h-i,3675a-i,3676a
TI Tricyclic compounds in which naphthalene is joined by "ortho fusion"
with a heterocyclic compound
AU Fries, K.; Walter, R.; Schilling, K.
SO Ann. (1935), 516, 248-85
AB The heats of combustion of anthracene and phenanthrene were detd. to be
9483.9 \pm 1.03 cal./g. and 9457.7 \pm 0.84 cal./g., resp.; the heats of
evapn. were calcd. to be 12.8 and 12.6 kg. cal. per mole, resp. 2,6-
C14H8(OH)2 and Br in dioxane give the 1,5-di-Br deriv., greenish yellow,
decompg. 135°; di-Me ether, yellow, m. 280° (decompn.); oxidation with
CrO3 in AcOH gives 1,5-dibromo-2,6-dimethoxyanthraquinone, yellow,
decompg. 345°; its structure was established by synthesis from 2,3-Br
(MeO)C6H3CO2H by heating with P2O5. lin-Naphthotriazole [(2',3',5,4)-

naphtho-(1,2,3-triazole)] (I) gives an Ac deriv., pale yellow, m. 149°; the 1-Me deriv., prepd with alk. Me₂SO₄, m. 175°. Reduction of I with Na-Hg in boiling EtOH gives the 8,9-dihydride (II), m. 157°; N-Me compd., m. 147°; N-Ac compd., m. 173°. Catalytic reduction of I (18 hrs.) gives the 4,5,6,7-tetrahydride (III), m. 162°; N-Ac deriv., m. 114°; N-Me deriv., m. 99°; II is only very slowly further catalytically reduced; angular naphthotriazole (IV) is only very slightly catalytically reduced. I, II or III on oxidation give lin-naphthotriazole-8,9-quinone (V), yellow, m. 242° (decompn.); it does not react with PhNH₂ in boiling EtOH; N-Ac deriv., pale yellow, m. 186°; N-Me compd., pale yellow, m. 237°. Reduction of V in Ac₂O gives the tri-Ac deriv. of lin-8,9-dihydroxynaphthotriazole, yellow, m. 165°. I and Cl in AcOH give the 8,9-di-Cl deriv., yellow, m. 291° (decompn.); oxidation gives V. I and Br in AcOH give the 9-Br deriv., bright reddish brown, m. 244° (decompn.); twice as much Br gives the 8,9-di-Br deriv., pale brownish yellow, m. 278° (decompn.); oxidation gives V. I and HCHO in EtOH give the 1-methylol deriv. decomp. 191° with evolution of HCHO and formation of I; it is also decompd. by soln. in dil. NH₄OH or by concd. H₂SO₄. I and ClCH₂CO₂Na in dil. NaOH, refluxed 5 hrs., give the 1-acetic acid deriv., yellow, m. 229°; it is pptd. unchanged from concd. H₂SO₄; heating decomposes it into CO and the 1-Me deriv. of I. I and ClCH₂COCl in boiling C₆H₆ give 90% of the 1-chloroacetyl deriv., greenish yellow, m. 179°; concd. H₂SO₄ gives a citron-yellow soln.; with AlCl₃ in PhNO₂ there results lin-naphthomorpholone, m. 270°; this also results from condensation of 2,3-H₂NC₁₀H₆OH and ClCH₂CO₂H. The heats of combustion of I and IV are 7369.3 ± 0.56 cal./g. and 7349.9 ± 1.02 cal./g., resp. 2,3-C₁₀H₆(NH₂)₂ and HCO₂H, refluxed 1 hr., give nearly quant. lin-naphthimidazole (VI), m. 221°; N-Ac deriv., m. 172°; oxidation of VI gives 70% of the 8,9-quinone (VII), yellow or brown-yellow, m. above 400°; NaOH gives an orange-yellow salt; it is repptd. unchanged from concd. H₂SO₄; it does not react with PhNH₂ in boiling EtOH; the Me deriv., light yellow, m. 286°; reduction of VII with Zn in Ac₂O gives the tri-Ac deriv. of 8,9-di-hydroxy-lin-naphthimidazole, m. 216°. 2,3-C₁₀H₆(NH₂)₂ and AcOH, heated 4 hrs. give the 2-Me deriv. of VI, m. 286°; its 8,9-quinone, yellow, m. above 350°; the Na salt is orange-red; it does not react with PhNH₂. The di-Ac deriv. of 1,2-H₂NC₁₀H₆OH with Ac₂O gives the tri-Ac deriv., m. 119.5° (Grandmougin, Ber. 39, 2495 (1906), believed this to be a polymer of the di-Ac deriv.); heating at 240-50° gives 2-methyl-2', 1'-naphthoxazole (VIII), b. 312°; the 1',2'-isomer (IX), b. 302°, m. 41.5°; the 2',3'-isomer (X), b. 310°, m. 87.5°, results from the di-Ac deriv. of 3,2-H₂NC₁₀H₆OH, m. 188°, by heating at 258°. The heats of combustion are: VIII 7778.7 ± 1.8 cal./g.; IX 7729.8 ± 6.4 cal./g.; X 7775.8 ± 4.9 cal./g. The following work was undertaken in an effort to prep. 2,3-C₁₀H₆(NH₂)₂ by a new method. 2,3-H₂NC₁₀H₆CO₂H (5.6 g.) and 15 cc. AcOH, on refluxing, give 5.5 g. dehydro-2-acetylamino-3-naphthoic acid (XI), m. 173°; heating with AcOH gives the known mono-Ac deriv., which yields XI with Ac₂O. XI and N₂H₄.H₂O in EtOH give 88% of 2-acetylamino-3-naphthoic acid hydrazide (XII), m. 225° (decompn.); the free NH₂ deriv., yellowish green, m. 206-10° (decompn.), results from 2,3-H₂NC₁₀H₆CO₂Me or better from linear benzoisatoic anhydride with N₂H₄.H₂O. XII and dil. HCl give 2-acetylamino-2-naphthoic acid azide (XIII), yellow, m. 233° (explosion). Heating XIII in C₆H₆ gives N-acetyl-2,3-naphthoimidazolone, m. 238°; heating XIII in AcOH gives the O-Ac isomer,